

1,3-Propanediol, diacetate  
628-66-0 | DTXSID30211889

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.03e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.37e-01

Confidence level: 7.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N-Methoxymethylamine</div> <div>Measured: 1.80e-01</div> <div>Predicted: 122</div>	<div>Image not found</div> <div>Hexamethyleneimine</div> <div>Measured: 7.74e-02</div> <div>Predicted: 15.0</div>	<div>Image not found</div> <div>Phenyl acetate</div> <div>Measured: 4.39e-02</div> <div>Predicted: 3.39e-01</div>
<div>Image not found</div> <div>Acetic acid, chloro-, 1-methylethyl ester</div> <div>Measured: 2.69e-01</div> <div>Predicted: 6.23</div>	<div>Image not found</div> <div>Fumaryl chloride</div> <div>Measured: 6.04e-02</div> <div>Predicted: 1.29</div>	